

# Interactions and Collisions of Discrete Breathers in Two-Species Bose-Einstein Condensates in Optical Lattices

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The dynamics of static and travelling breathers in two-species Bose-Einstein condensates in a one-dimensional optical lattice is modelled within the tight-binding approximation. Two coupled discrete nonlinear Schrödinger equations describe the interaction of the condensates in two cases of relevance: a mixture of two ytterbium isotopes and a mixture of  $^{87}\text{Rb}$  and  $^{41}\text{K}$ . Depending on their initial separation, interaction between static breathers of different species can lead to the formation of symbiotic structures and transform one of the breathers from a static into a travelling one. Collisions between travelling and static discrete breathers composed of different species are separated in four distinct regimes ranging from totally elastic when the interspecies interaction is highly attractive to mutual destruction when the interaction is sufficiently large and repulsive. We provide an explanation of the collision features in terms of the interspecies coupling and the negative effective mass of the discrete breathers.

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## I. INTRODUCTION

Bose-Einstein condensates have become a formidable tool for studying basic fundamentals of atomic physics [1, 2]. When confined to an optical lattice they serve as an interesting analogue to a solid-state system [3, 4], providing means to study solid-state phenomena at an unprecedented level of parameter control. These include quantum phase transitions from the superfluid to Mott-insulator regimes [5], transport phenomena [6], Anderson localization [7], low-dimensional systems [8], discrete breathers [9] and solitons [10]. The latter can exist both with or without a periodic potential, although a lattice environment makes it possible for solitons and discrete breathers to exist even when the interactions in the BEC are repulsive (“gap solitons”) [11–13]. Such states have been observed experimentally in [14]. Several other methods have been proposed in the literature, including the use of an additional harmonic potential [15] and boundary dissipations [16], which could also be used for non-demolition probing of these states [17].

The introduction of a second atomic species, i.e. the creation of a binary mixture of Bose-Einstein Condensates leads to even richer physics. In a harmonic trap the two species may be immiscible due to the interspecies interaction, leading to phase separation [18, 19]. In an effectively one-dimensional environment, the repulsive interaction between atoms of different species (‘interspecies’ interactions) during the formation of the condensate can leave the mixture far from its ground state [20, 21]. The interspecies interactions heavily influence the transport properties of a condensate in a lattice [22, 23]. Repulsive interactions enable the formation and ex-

tend the stability region of the so-called *symbiotic* gap solitons [24–26], i.e. two-species solitons localized together in the same spot of the lattice. Somewhat counter-intuitively, an attractive interspecies interaction may split the two overlapping solitons [27].

So far most of the work has concentrated on the existence of two-species solitons and their stability [24–31]. In this paper we take a complementary approach – we start with well-defined single-species discrete solitons (two travelling breathers or a self-trapped state and a travelling breather, the first made of one species and the other of the second species) far apart in the lattice and simulate their collisions. For a single species BEC confined to a one-dimensional lattice collisions of travelling breathers have been analyzed in detail in [32]. Such an approach has also been used in the case of binary BECs in harmonic traps [33, 34]. We perform our simulations using experimentally reachable conditions, with specific reference to two feasible experiments of two-species BECs in optical lattices.

The first of these experiments of interest has been performed in Kyoto where BECs of Yb atoms have been obtained separately with isotopes  $^{174}\text{Yb}$  [35] and  $^{170}\text{Yb}$  [36], as well as a mixture of isotopes  $^{174}\text{Yb}$  and  $^{176}\text{Yb}$  [37] (see also [38]).

In the mixture case, however, the latter component quickly collapses due to its negative intraspecies scattering length. The intra- and interspecies scattering lengths of ytterbium isotopes have been measured using data from one- [39] and two-color photoassociation spectroscopy [40] and are now well established. The rich isotope structure of ytterbium enables mass tuning of the scattering length. It has been shown that, unlike in alkali-metal species, optical Feshbach resonances can be used to effectively change the intraspecies scattering length [41–43], thus raising hope for optical control of interactions between different isotopes. Three bosonic isotopes of ytterbium, namely  $^{168,170,174}\text{Yb}$  have positive intraspecies

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scattering lengths of the order of a few nanometers leading to similar stable condensates. Since the isotope shifts are small compared to the detuning of the far off resonant trap (FORT), the potential seen by different isotopes is basically identical.

Even though these three isotopes are similar in terms of the single-species scattering length, the interspecies interactions of different pairs of isotopes differ dramatically. The interaction between a  $^{170}\text{Yb}$  and  $^{174}\text{Yb}$  atoms is described by a large negative scattering length of -27.3 nm, while for  $^{168}\text{Yb}$  and  $^{170}\text{Yb}$  it is positive and equal to 6.2 nm. Halfway between these two is the case of  $^{168}\text{Yb}$  and  $^{174}\text{Yb}$  characterised by a negligible scattering length of 0.13(18) nm, where the two condensate species should essentially ignore each other.

Recently, an interesting mixture of heteronuclear BECs has been obtained in an experiment of Thalhammer et al. [44], where  $^{41}\text{K}$  and  $^{87}\text{Rb}$  atoms are condensed together in an optical lattice. A remarkable property of this mixture is that the interspecies scattering length  $a_{1,2}$  describing the effective interaction of colliding potassium and rubidium atoms can be tuned over a wide (both positive and negative) range using a magnetic Feshbach resonance, while the single-species scattering length remains positive for either species.

We present an analysis of the interaction and collisional behavior of discrete breathers in two-species BEC in optical lattices in the tight-binding approximation which has been successfully used to describe single-species experiments [9, 11, 12, 45]. In Section II the derivation of the model and an estimate of the parameters are provided. Interaction of stationary breathers in close proximity to each other is described in section III. Collision of traveling breathers and trapped states are described in Section IV as a function of the interspecies coupling parameter. Section V provides an explanation of the different kind of collisions observed in the numerical simulations where inelastic behavior is found in the mutually-repulsive case and elastic in the mutually-attractive case.

## II. THE TIGHT-BINDING APPROXIMATION APPLIED TO A TWO-SPECIES BOSE GAS

We analyze the behavior of the two-species Bose gas with the use of the tight-binding approximation, following the treatment described in [23]. The time-dependent Gross-Pitaevskii equations describing the dynamics of the two species' order parameters  $\Psi_i$  (where  $i = 1, 2$ ) read

$$i\hbar\Psi_i(\vec{r}) = \left( -\frac{\hbar^2}{2m_i}\nabla^2 + U(\vec{r}) + \sum_{j=1,2} g_{i,j}|\Psi_j(\vec{r})|^2 \right) \Psi_i(\vec{r}), \quad (1)$$

where the coefficients  $g_{i,j}$  describe the effective mean-field intra- and interspecies interactions and are given by

$$g_{i,j} = \frac{4\pi\hbar^2 a_{i,j}}{2\mu_{i,j}}, \quad (2)$$

where  $\mu_{i,j} = (m_i^{-1} + m_j^{-1})^{-1}$  is the reduced mass of the atomic pair and  $a_{i,j}$  is the scattering length relevant in the scattering properties of the species' atoms.

The external potential confining the BECs is due to two overlapping and counter-propagating laser beams that create a standing wave in the axial direction and, as a result, a periodic potential of depth  $V_{0,i}$ . The Gaussian profile of the two laser beams gives rise to an approximately harmonic off-axis confinement described by the frequencies  $\omega_{r,i}$ . Thus the external potential reads

$$V_i = V_{0,i} \sin^2(kx) + \frac{1}{2}m_i\omega_{r,i}^2(y^2 + z^2). \quad (3)$$

Note that real optical lattices also have a shallow harmonic potential superimposed in the axial direction, which we here assume to have negligible effects. We also introduce the lattice strengths  $s_i = V_{0,i}/E_{R,i}$ , where  $E_{R,i} = \hbar^2 k^2 / 2m_i$  is the recoil energy calculated for the lattice wavelength. The axial on-site frequency of the lattice is then  $\omega_i = \sqrt{s_i} \hbar k^2 / m_i$ .

Both order parameters obey the normalisation condition  $\int d^3\vec{r} |\Psi_i|^2 = N_i$ , where  $N_i$  denotes the total number of atoms of the  $i$ -th species in the lattice.

If the lattice is strong enough, i.e. the trap depth is sufficiently large, the condensate is well localised around potential minima. For each of the mixture's order parameters we use the following *ansatz* [11, 23, 30]:

$$\Psi_i = \sum_n \psi_{i,n}(t) \phi_i(\vec{r} - \vec{r}_{i,n}), \quad (4)$$

where  $\phi_i$  is an on-site wavefunction and  $\vec{r}_{i,n}$  is the location of the  $n$ -th lattice site seen by the  $i$ -th species. When the atomic interactions are weak, the on-site ground state wavefunction can be replaced by the ground state harmonic oscillator wavefunction in the off-axis direction and a Wannier function [46] of the lowest band in the axial direction to account for tunneling. Consequently,  $|\psi_{i,n}(t)|^2$  may be interpreted as the number of  $i$ -th species atoms in the  $n$ -th lattice site as a function of time and  $\sum_n |\psi_{i,n}|^2 = N_i$ .

Substituting this *ansatz* into the Gross-Pitaevskii equations and dropping all terms mixing different lattice sites except for the ones that describe tunneling (see [11, 23]) one obtains

$$i\hbar\dot{\psi}_{i,n} = -J_i(\psi_{i,n-1} + \psi_{i,n+1}) + (\lambda_{i,i}|\psi_{i,n}|^2 + \lambda_{1,2}|\psi_{3-i,n}|^2 + \epsilon_{i,n})\psi_{i,n} \quad (5)$$

where

$$J_i = \int d^3\vec{r} \phi_i(\vec{r} - \vec{r}_{i,n}) \left( \frac{-\hbar^2}{2m_i} \nabla^2 + V_i \right) \phi_i(\vec{r} - \vec{r}_{i,n+1}) \quad (6)$$

is the hopping integral describing the tunneling of the  $i$ -th species and is proportional to the intersite tunneling rate  $\gamma_i = J_i/\hbar$ , while  $\epsilon_{i,n} = \int d^3\vec{r} \phi_i(\vec{r} - \vec{r}_{i,n}) \left( \frac{-\hbar^2}{2m_i} \nabla^2 + V_i \right) \phi_i(\vec{r} - \vec{r}_{i,n})$  is the on-site chemical potential. The self- and mutual interaction is described by the parameters  $\lambda_{i,i} = g_{i,i} \int d^3\vec{r} |\phi_i(\vec{r})|^4$  and  $\lambda_{1,2} = g_{1,2} \int d^3\vec{r} |\phi_1(\vec{r})|^2 |\phi_2(\vec{r})|^2$ , respectively.

### A. Normalization

In order to move towards a more standard and computationally efficient form of two coupled discrete nonlinear

TABLE I: Values of parameters used in the simulations

Pair	$s_1$	$s_2$	$\gamma_2/\gamma_1$	$\Lambda_{1,1}$	$\Lambda_{2,2}$	$\Lambda_{1,2}$
$^{168}\text{Yb} + ^{170}\text{Yb}$	3.19	3.27	0.96	5.28	1.368	2.51
$^{170}\text{Yb} + ^{174}\text{Yb}$	3.27	3.43	0.91	1.368	2.486	-12.24
$^{87}\text{Rb} + ^{41}\text{K}$	3.03	7	6.97	12.31	5.89	(free)

Schrödinger equation (DNLSE), we introduce

$$z_{i,n} = \sqrt{\frac{1}{N_i}} \psi_{i,n}^* \exp\left(-i \frac{\epsilon_i \tau}{\hbar \gamma_1}\right) \quad (7)$$

$$\tau = \gamma_1 t \quad (8)$$

to obtain:

$$i \frac{d}{d\tau} z_{1,n} = \Lambda_{1,1} |z_{1,n}|^2 z_{1,n} + \Lambda_{1,2} \frac{N_2}{N_1} |z_{2,n}|^2 z_{1,n} - z_{1,n-1} - z_{1,n+1} \quad (9)$$

$$i \frac{d}{d\tau} z_{2,n} = \Lambda_{2,2} |z_{2,n}|^2 z_{2,n} + \Lambda_{1,2} |z_{1,n}|^2 z_{2,n} - \frac{\gamma_2}{\gamma_1} (z_{2,n-1} + z_{2,n+1}). \quad (10)$$

In Eqs. (9-10) we have defined the following parameters:

$$\Lambda_{i,i} = \frac{\lambda_{i,i} N_i}{\hbar \gamma_1} \quad \Lambda_{1,2} = \frac{\lambda_{1,2} N_1}{\hbar \gamma_1}. \quad (11)$$

Thus the atomic distribution of each species over the entire lattice is normalized to unity:

$$\sum_n |z_{i,n}|^2 = 1. \quad (12)$$

To ensure that the energy and density in the system are conserved, we use a symplectic fourth-order integrator of the Yoshida type [47, 48]. The energy and density are both conserved up to 9 decimal places at each integration time step.

### B. Estimate of the calculation parameters

In Section III(A) we present results that model different Bose gas mixtures, notably mixtures of ytterbium isotopes and that of  $^{41}\text{K} + ^{87}\text{Rb}$ . At present, the only ytterbium isotope mixture BEC obtained so far is that of  $^{174}\text{Yb} + ^{176}\text{Yb}$  where, however, the  $^{176}\text{Yb}$  part instantly collapses because of its negative scattering length [37]. Thus we focus on ytterbium mixtures of isotopes whose scattering length is positive, namely  $^{168}\text{Yb}$ ,  $^{170}\text{Yb}$  and  $^{174}\text{Yb}$ . The latter two have already reached BEC separately [35, 36] while the major technical difficulty in reaching a  $^{168}\text{Yb}$  BEC is its low natural abundance of 0.13%.

To calculate the self nonlinear parameter,  $\lambda_{i,i}$ , it is sufficient to approximate the on-site wavefunction  $\phi_{i,n}(\vec{r})$  with a harmonic oscillator ground state, which is basically a Gaussian, to yield

$$\lambda_{i,i} = a_{i,i} \sqrt{\frac{m \omega_r^2 \omega}{2\pi \hbar}} \quad (13)$$

In the case of ytterbium mixtures the mutual interaction parameter  $\lambda_{1,2}$  can also be estimated from the above formula as the masses of the two isotopes are very similar and the two wavefunctions are well overlapped.

In the case of the  $^{41}\text{K} + ^{87}\text{Rb}$  mixture the two wavefunctions are differently shaped (one is narrower than the other due to the difference in masses). The difference in the masses of the two species has a further effect - the two clouds are separated due to gravity but an additional laser can be used to force overlap of the two species [49]. The scattering length of  $^{87}\text{Rb}$  is 5.25 nm [50] while for  $^{41}\text{K}$  it is 3.1 nm [51, 52]. The inter-species scattering length can be changed by the use of a convenient magnetic Feshbach resonance [53] so that  $\lambda_{1,2}$  can be considered as a free parameter.

To estimate the tunneling rates  $\gamma_i$ , it is not sufficient to approximate the on-site wavefunctions with Gaussians and one has to use the Wannier wavefunctions. This is because the tunneling rate is mostly determined by the wings of the on-site wavefunction which have an oscillatory-exponential rather than a Gaussian tail. In this case the tunneling rate can be approximated as [4]

$$J_i = \hbar \gamma_i = \frac{4}{\sqrt{\pi}} E_{r,i} s_i^{3/4} \exp(-2\sqrt{s_i}). \quad (14)$$

The parameters for the ytterbium isotopes considered here are as follows. The lattice laser wavelength is 532 nm; the lattice frequencies for both species are  $\omega_r = 2\pi \times 100$  Hz and  $\omega = 2\pi \times 15$  kHz which are close to the experimental realizations. For the sake of simplicity, we consider  $N_1 = N_2 = O(10^3)$  as it is difficult to find initial conditions that would lead to a *clear* traveling breather at larger densities. This is a general property of gap solitons [15]. The results apply, however, to larger values of  $N_i$  up to  $10^5$ .

In the case of the  $^{87}\text{Rb}$  and  $^{41}\text{K}$  mixture we consider a lattice wavelength of 1064 nm and we take the (tunable) lattice depth to be  $V_e = 7E_r$  for rubidium so that the same parameter for potassium is around 3. This is done to ensure that we can still use the tight-binding approximation (i.e. tunneling rates to further sites are at least an order of magnitude smaller than  $\gamma_i$ , see table I in [4]). On the other side the tunneling rate needs to be large enough for traveling breathers to exist.

The calculation parameters discussed above are shown in table I.

## III. BREATHING INTERACTION

It has been demonstrated that initially Gaussian wavepackets can evolve via the single species DNLSE into static breathers [9, 11, 45]. If the wavepacket is given a momentum in a certain direction, travelling breathers that translate across the lattice can also be formed. The general expression of the initial wavepacket is:

$$z_{i,n} = \sqrt{\frac{1}{\sqrt{2\pi\sigma_i^2}}} \exp\left(-\frac{(n - \bar{n}_i)^2}{4\sigma_i^2}\right) e^{ip_i n} \quad (15)$$

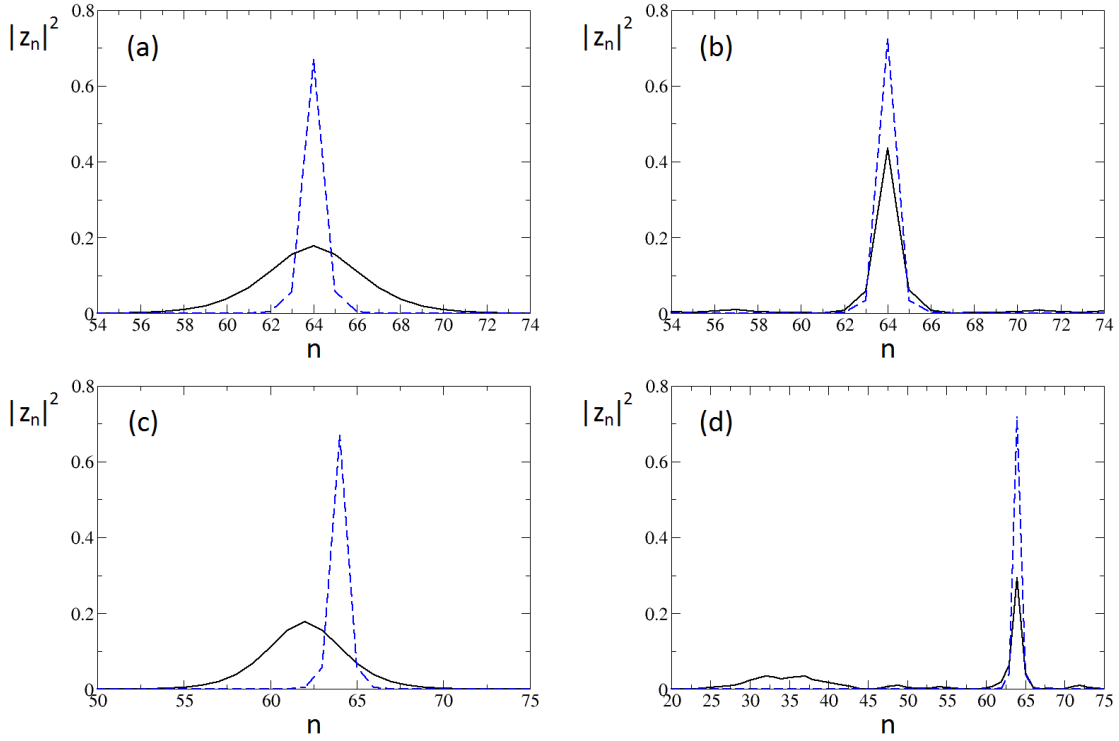


FIG. 1: (Color online) Density profiles of  $^{168}\text{Yb}$  (black solid line) +  $^{170}\text{Yb}$  (blue dashed line) mixture. (a) Initial density profile of  $^{168}\text{Yb}$  +  $^{170}\text{Yb}$  breathers with  $D = 0$ . (b) Density profile of  $^{168}\text{Yb}$  +  $^{170}\text{Yb}$  breathers at  $\tau = 1000$  after  $\Lambda_{1,2}$  is switched on for  $D = 0$ . Note that the density profiles have changed when forming the symbiotic breather. (c) Initial density profile of  $^{168}\text{Yb}$  +  $^{170}\text{Yb}$  breathers with  $D = 2$ . The wavefunctions of the two species still overlap significantly. (d) Density profile of  $^{168}\text{Yb}$  +  $^{170}\text{Yb}$  breathers at  $\tau = 1000$  after  $\Lambda_{1,2}$  is switched on for  $D = 2$ . Note that the  $^{168}\text{Yb}$  is smaller and some of the background has become localised to the left of the main breather.

where  $\sigma_i$  is the initial width of the Gaussian cloud, and  $\hat{n}_i$  is its position. For the single species case, low nonlinearity and values of  $|p_i|$  between zero and  $\pi/2$ , corresponding to a positive  $\cos p_i$ , the cloud expands diffusively within the lattice. Localization into static breathers is then observed when increasing the repulsive self-interaction  $\Lambda_{i,i}$ . However, when the pseudomomentum crosses  $\pi/2$  and the repulsive self-interaction  $\Lambda_{i,i}$  is not too large, travelling breathers are formed (unless  $\cos p_i$  is exactly 1, in which case the breather is stationary) [9, 11, 16, 17, 45, 54].

In this section, we run simulations starting from stationary breathers of  $^{168}\text{Yb}$  and  $^{170}\text{Yb}$  in separate positions. These are formed by running simulations of initially Gaussian wavepackets with  $\Lambda_{1,2} = 0$  and letting them reshape with dissipation applied at the boundaries to get rid of the background (see [9] for a detailed description of the effects of dissipation). Once the breathers are formed and the background noise has vanished, we turn dissipations off and set  $\Lambda_{1,2}$  to the value of 2.51.

For each simulation, we change the initial distance  $D$  between the centres of the single-species breathers and then study the breather interaction. With the stationary breathers centred on the same site at the start of the simulation ( $D = 0$ ), a symbiotic breather is formed, with the  $^{168}\text{Yb}$  breather ex-

pulling excess atomic density into the background (see Fig. 1 (a) and (b)). The density profile of the symbiotic breather is then different than that of the two breathers occupying the same site with  $\Lambda_{1,2} = 0$ .

This behaviour keeps occurring when the initial distance between the breathers is larger, but still small enough that the density profiles overlap significantly. An example of this behavior is shown in Fig. 1 (c) and (d), for  $D = 2$ . Here, we see that less of the  $^{168}\text{Yb}$  atoms join with the symbiotic breather and more are expelled into the background. A small travelling breather is then formed from the atoms in the background. The reshaping process of the  $^{170}\text{Yb}$  breather is much the same as with  $D = 0$ .

The formation and evolution of a traveling breather out of the interaction of two static breathers of separate species is shown more clearly in Fig. 2, in which we see that the traveling breather reflects off the nearest boundary and then off the breather in the center of the lattice. In all simulations we consider that lattice sites outside the condensate are empty resulting in reflective boundaries. This is realized experimentally by fixing the size of the condensate with external magnetic fields. This is why breathers are observed to “bounce” off the boundaries in many figures of the paper. With  $D = 8$ , the example shown in Fig. 2(a), the initial density profiles of the

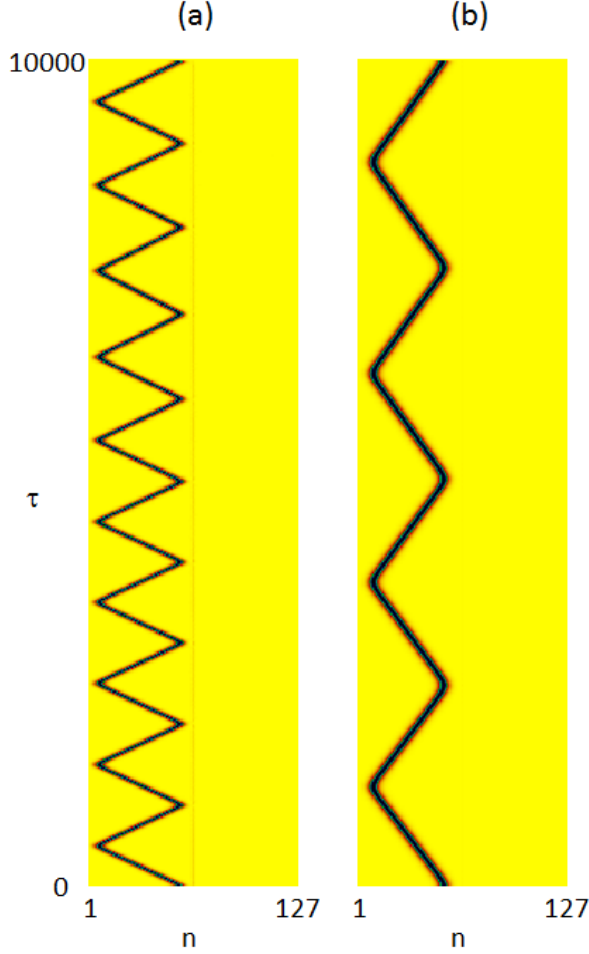


FIG. 2: (Color online) Interaction between initially stationary breathers in the  $^{168}\text{Yb} + ^{170}\text{Yb}$  mixture for (a)  $D = 8$  and (b)  $D = 11$ . Both images show only the evolution of the  $^{168}\text{Yb}$  part of the mixture since the  $^{170}\text{Yb}$  evolution is rather straightforward, with the breather highly localised in the centre. The majority of  $^{168}\text{Yb}$  atoms forms a travelling breather while the remaining atomic density is absorbed by the  $^{170}\text{Yb}$  breather to form a symbiotic breather. The travelling breather reflects off the nearest boundary and then off the  $^{170}\text{Yb}$  breather in the centre of the lattice.

breathers only overlap at the tails. The result of this is that only a small density of  $^{168}\text{Yb}$  atoms contributes to the symbiotic breather. As  $D$  is increased, more  $^{168}\text{Yb}$  atoms go into the travelling breather and less in the symbiotic one. In Fig. 2(b), for  $D = 11$ , we see that the symbiotic breather is not formed anymore and the travelling breather is denser, and slower, than that formed for  $D = 8$  (Fig. 2(a)). This is due to the initial density profile for  $D = 11$ , in which the breathers do not overlap any longer. It is important to stress that the motion of the travelling breather made of  $^{168}\text{Yb}$  atoms is due to the interaction of the two species via  $\Lambda_{1,2}$  being different from zero. In the case of no-interaction ( $\Lambda_{1,2} = 0$ ) both breathers remain stationary at all times. For all these examples, the evolution of the  $^{170}\text{Yb}$  breather is very similar to the case of  $D = 0$ , with the high localisation in the centre of the lattice and minimal

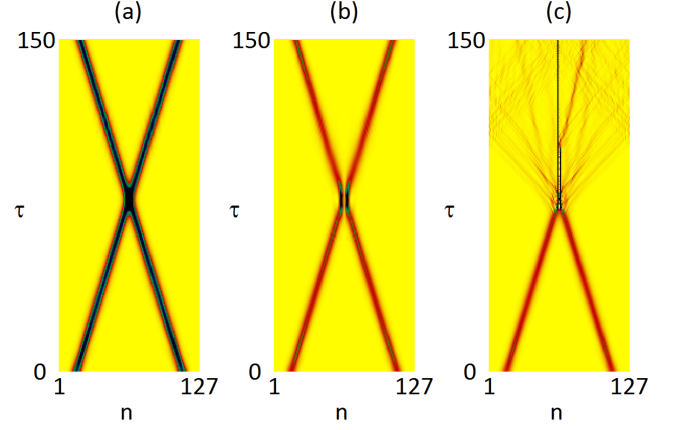


FIG. 3: (Color online) Collision of two traveling breathers in the  $^{170}\text{Yb}$  (left) +  $^{174}\text{Yb}$  (right) mixture. The initial conditions are  $\Lambda_1 = \Lambda_2 = 1.1$ ,  $\bar{n}_1 = 16$ ,  $\bar{n}_2 = 112$ ,  $\sigma_1 = \sigma_2 = 3$  and  $\cos p_1 = \cos p_2 = -0.95$  for all panels. Note that  $p_1 = -p_2$  and therefore the traveling breathers move in opposite directions.  $\Lambda_{1,2} = 0$  is set to: (a) 0, (b) 0.2 and (c) 0.3. In (a), the breathers ignore each other acting as if the other species was not present. In (b), the breathers collide elastically. In (c), the breathers are destroyed and a new symbiotic breather is created.

background noise.

#### IV. COLLISION OF TRAVELLING AND STATIONARY BREATHERS

Having assessed the interaction of discrete breathers of different atomic species when set in close proximity, we investigate here the collision of these breathers having set one or both of them in motion by using the pseudomomentum  $p_i$  in the initial conditions given by (15). Experimentally, traveling breathers can be constructed by accelerating the lattice confining the condensate. Such accelerations were realised experimentally in [55] while observing optical lensing effects. In the case of two different species in the same lattice the difference in the masses will naturally lead to different pseudomenta of the clouds after acceleration to the same group velocity, thus making collisions possible.

In Fig. 3, we show three symplectic simulations of two colliding traveling breathers, with carefully chosen parameters so that there would be a minimal amount of sound-waves emitted from the initial Gaussian distributions. In all simulations presented in Fig. 3 the breathers start from the same initial conditions but with different values of the interspecies interaction parameter  $\Lambda_{1,2}$ . The color represents the (normalized) atomic density  $|z_{n,i}|^2$  with  $i = 1$  for one species and  $i = 2$  for the other. The simulations start with two Gaussian wavepackets of the form (15) with  $\cos p_1 = \cos p_2 = -0.95$  and  $p_1 = -p_2$  to form two colliding traveling breathers.

In Fig. 3(a) when the interspecies interaction parameter  $\Lambda_{1,2}$  is set to zero, the breathers follow the dynamics of single-species condensates. They are unaffected by the others presence and pass through each other. When  $\Lambda_{1,2}$  is a non-zero



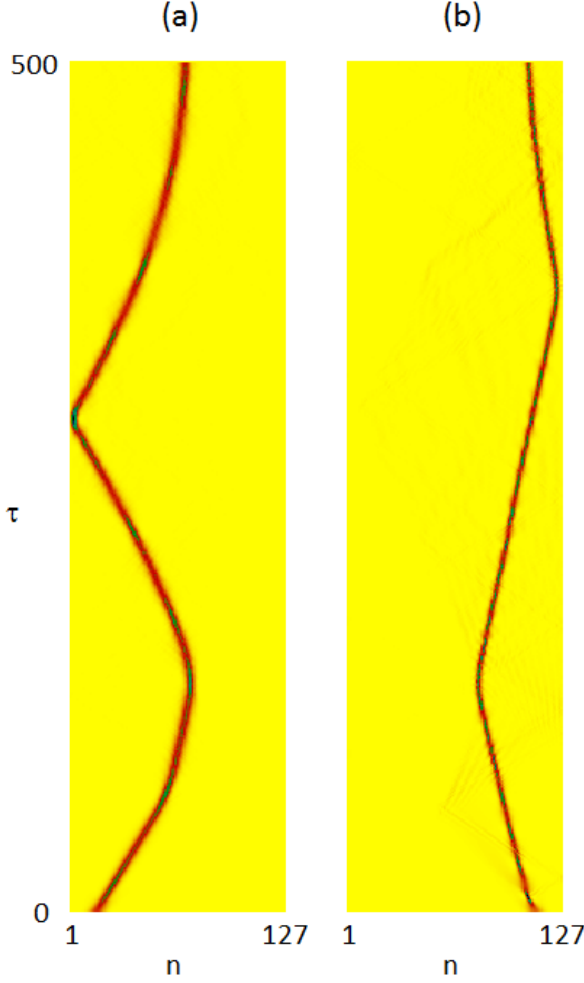


FIG. 4: (Color online) A collision of two traveling breathers in the  $^{170}\text{Yb}$  (a) +  $^{174}\text{Yb}$  (b) mixture characterised by a large negative interspecies scattering length of  $-27.3$  nm. The Gaussian parameters for the initial condition are  $\bar{n}_1 = 16$ ,  $\bar{n}_2 = 112$ ,  $\sigma_1 = \sigma_2 = 3$  and  $\cos p_1 = \cos p_2 = -0.95$ . The collision is elastic.

value, the two species affect each other when occupying the same lattice sites. This is shown in Fig. 3(b) and (c). At the beginning of the simulations, when the breathers are far apart from one another in the lattice, they follow the same path as in Fig. 3(a), until they collide. For large negative values of  $\Lambda_{1,2}$ , the breathers collide elastically, as shown in figure 3(b). In this example,  $\Lambda_{1,2} = -20$  and the breathers become narrower when they collide. In Fig. 3(c),  $\Lambda_{1,2}$  is changed to a positive value and the collision is not elastic. At the collision, the breathers explode, emitting a large amount of sound waves and a stationary symbiotic soliton composed of both species is formed.

It is worth noting that elastic collision occurs when the interspecies interaction parameter is negative, which would normally imply *attractive* interactions between the two species. Normally the two clouds try to achieve maximal overlap in order to minimize energy, while in our case the tendency is to minimize the overlap and retain separation of at least a few

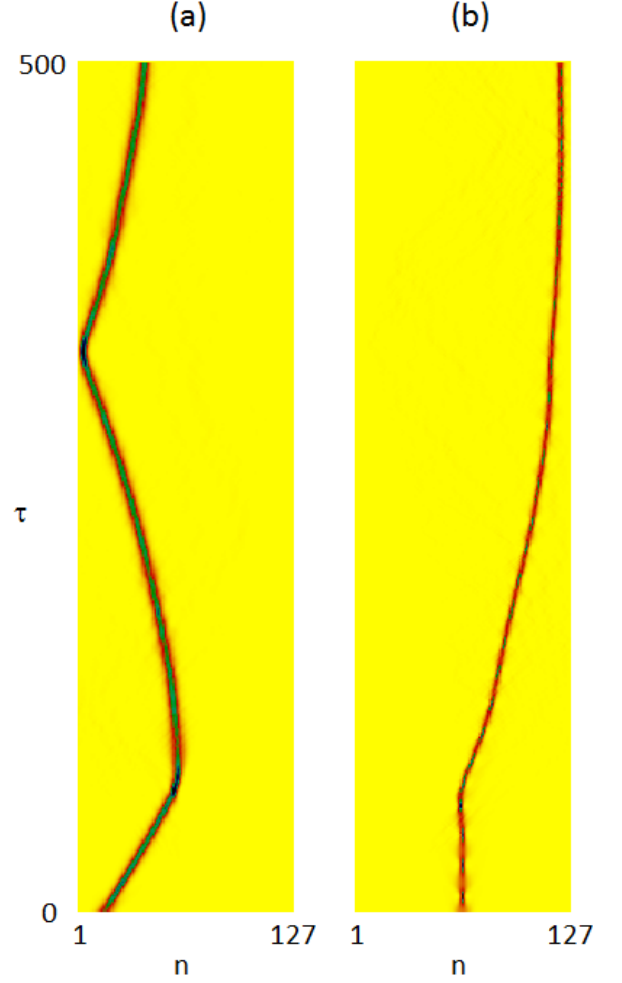


FIG. 5: (Color online) A collision of a traveling breather (a) with a stationary breather (b). The physical situation is the same as in Fig. 4, except that  $\bar{n}_2 = 64$  and  $\cos p_2 = -1$  to make a stationary breather. The traveling breather transfers large part of its (pseudo)momentum to the stationary one and nearly stops.

lattice sites. An explanation of this phenomenon by using the negative effective mass of the discrete breathers is provided in Section V.

For the simulations in Fig. 3, we have carefully chosen the parameters so that the amount of sound-waves emitted from the breathers is minimal. In the following we turn our attention to values of the parameters chosen from table I to model mixtures of ytterbium isotopes and that of  $^{41}\text{K} + ^{87}\text{Rb}$  in realistic configurations. In these simulations, although the initial condition emits large amount of noise, we show that the main dependence of the collision from the interaction parameter  $\Lambda_{1,2}$  remains that displayed in Fig. 3.

In Fig. 4 we show a numerical simulation of two colliding traveling breathers in the  $^{170}\text{Yb} + ^{174}\text{Yb}$  mixture that displays similar results to that of Fig. 3. Note that for all following simulations, the dynamics of each species is shown in separate panels, unlike Fig. 3. For example Fig. 4(a) shows the  $^{170}\text{Yb}$  species, while Fig. 4(b) shows the  $^{174}\text{Yb}$  species. At about

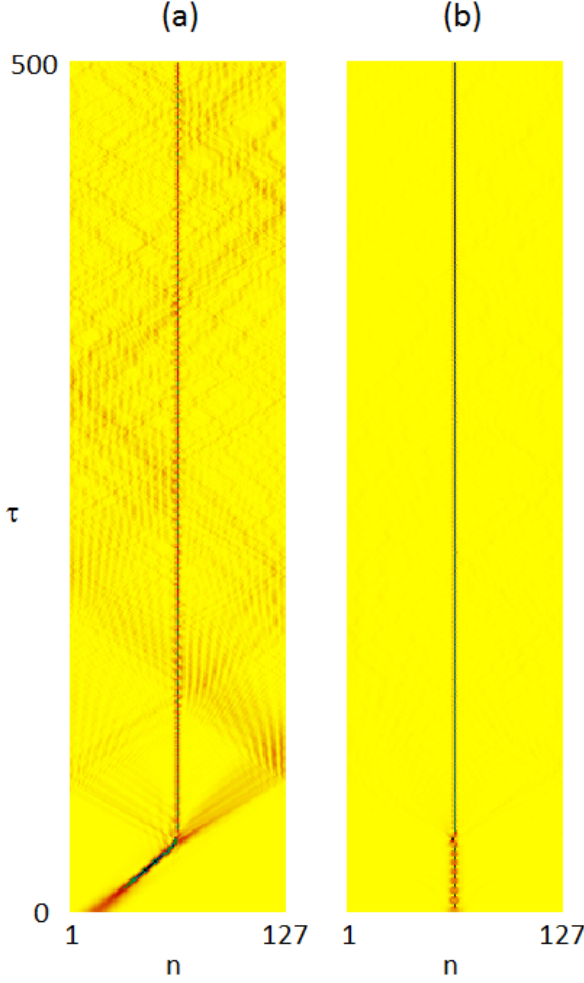


FIG. 6: (Color online) A collision of a traveling breather ( $^{170}\text{Yb}$ , shown in (a)) and a stationary breather ( $^{168}\text{Yb}$ , shown in (b)) for a positive interspecies scattering length of 6.2 nm. The initial condition parameters are  $\bar{n}_1 = 16$ ,  $\bar{n}_2 = 64$ ,  $\sigma_1 = 5$ ,  $\sigma_2 = 3$ ,  $\cos p_1 = 0.8$ ,  $\cos p_2 = 1.0$ . As in Fig. 3(c), the traveling breather is destroyed and a new *symbiotic* soliton is created.

$\tau \approx 90$  the two breathers collide elastically, as in Fig. 3(b) since the interspecies scattering length is large and negative.

Figure 5 shows a similar situation, except that now one of the breathers ( $^{174}\text{Yb}$ ) is at first stationary ( $\cos p_2 = -1$ ). After the collision the initially traveling breather (almost) stops while the other, up to now stationary, starts traveling. One could argue that this is a manifestation of a form of conservation of momentum. Again, as in Fig. 3, the elastic behaviour occurs even though the  $^{170}\text{Yb}$  and  $^{174}\text{Yb}$  pair is described by a large negative scattering length of  $a_{1,2} = -27.3$  nm, which, under normal circumstances, stands for *attraction* between the atoms of the two species.

Compared to the examples in Fig. 3, there is a much larger amount of sound waves emitted from the breathers in Figs. 4 and 5 due to the parameter values used from Table I. These small-amplitude sound waves do not appear to affect the main collision in a significant way and, in fact, a careful examina-

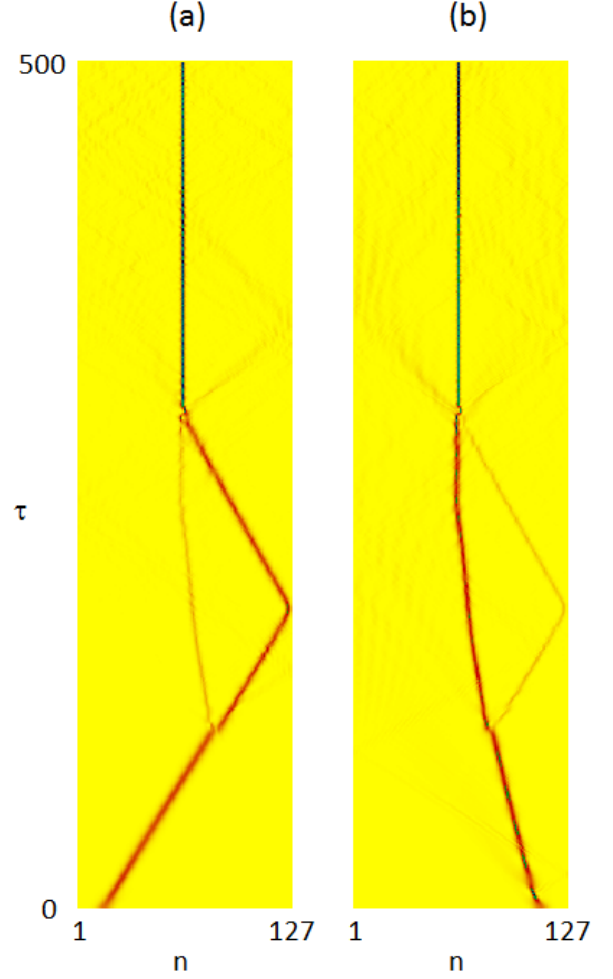


FIG. 7: (Color online) The same physical situation as in Fig. 4, except that the parameter  $\Lambda_{1,2}$  describing the interspecies has now been increased to 4, corresponding to a positive interspecies scattering length of 8.9 nm. In this regime, the two breathers tunnel through each other. Note that a small part of each breather is trapped inside the other forming double-species traveling breathers.

tion shows that the location of a breather of a certain species acts as an effective barrier to the sound waves of the other species emitted during the formation of the breathers. Sound waves that would normally expand over the entire lattice are now confined to a region limited by the position of the other-species breather.

A qualitatively different behavior from the above and similar to that in Fig. 3(c), is found in the case of the  $^{168}\text{Yb} + ^{170}\text{Yb}$  pair described by a positive (*repulsive*) scattering length of  $a_{1,2} = +6.2$  nm. Due to the large intraspecies interaction of  $^{168}\text{Yb}$  it is difficult to construct a clear traveling breather and therefore we limit ourselves to the case where the  $^{168}\text{Yb}$  breather is initially stationary. This situation is presented in Fig. 6. As in Fig. 3, at the time of impact ( $\tau \approx 40$ ) the two breathers literally explode emitting a large amounts of sound waves and forming a double-species symbiotic stationary breather. In this state, the two component wavefunctions

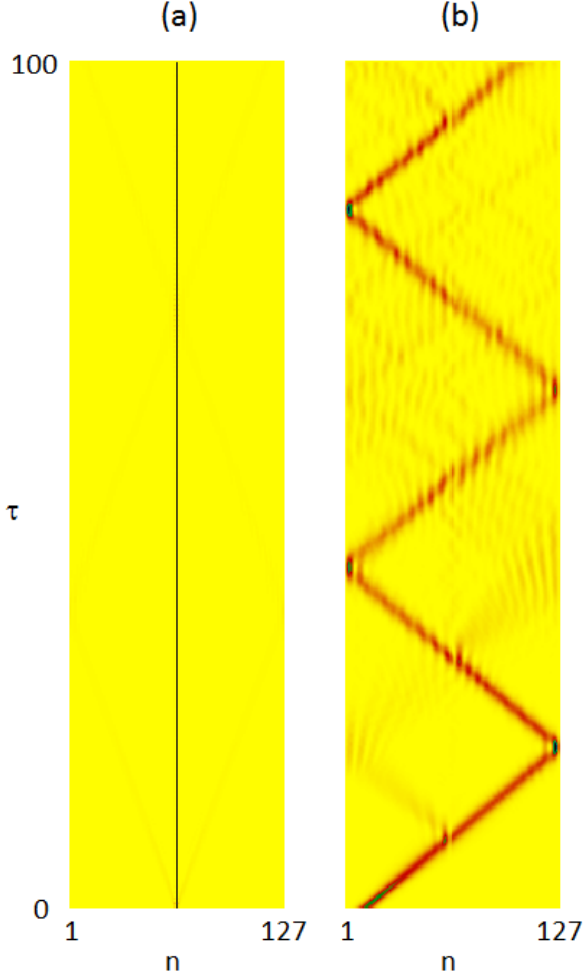


FIG. 8: (Color online) A collision of a traveling ( $^{41}\text{K}$ , shown in (b)) and a stationary breather ( $^{87}\text{Rb}$ , shown in (a)), with the interspecies interaction parameter  $\Lambda_{1,2} = 3$ . The initial condition parameters are  $\bar{n}_1 = 64$ ,  $\bar{n}_2 = 12$ ,  $\sigma_1 = 0.5$ ,  $\sigma_2 = 3$ ,  $\cos p_1 = 1$ ,  $\cos p_2 = -0.9$ . The traveling breather tunnels almost completely through the self-trapped state.

are well overlapped. Moreover, the final breather is much narrower than any of the original breathers before the collision. The frequency of oscillation of the two final co-located and co-existing breathers is species dependent. In the case displayed in Fig. 6 the frequency of the  $^{168}\text{Yb}$  breather is about 1.5 times that of the  $^{170}\text{Yb}$  breather located on the same site.

To further explore these phenomena we carried out a simulation for the physical situation described in Fig. 4 of the  $^{170}\text{Yb} + ^{174}\text{Yb}$  mixture but with the interaction parameter  $\Lambda_{1,2}$  increased to 4 corresponding to an interspecies scattering length of  $a_{1,2} = 8.9$  nm. Such an increase can potentially be achieved using an optical Feshbach resonance. In this situation, we observe the collision of two traveling breathers with a positive interspecies interaction as shown in Fig. 7. We find yet another collision behavior with these parameters: the two breathers mainly tunnel through each other but at each collision a fraction of the atomic species in one soliton becomes

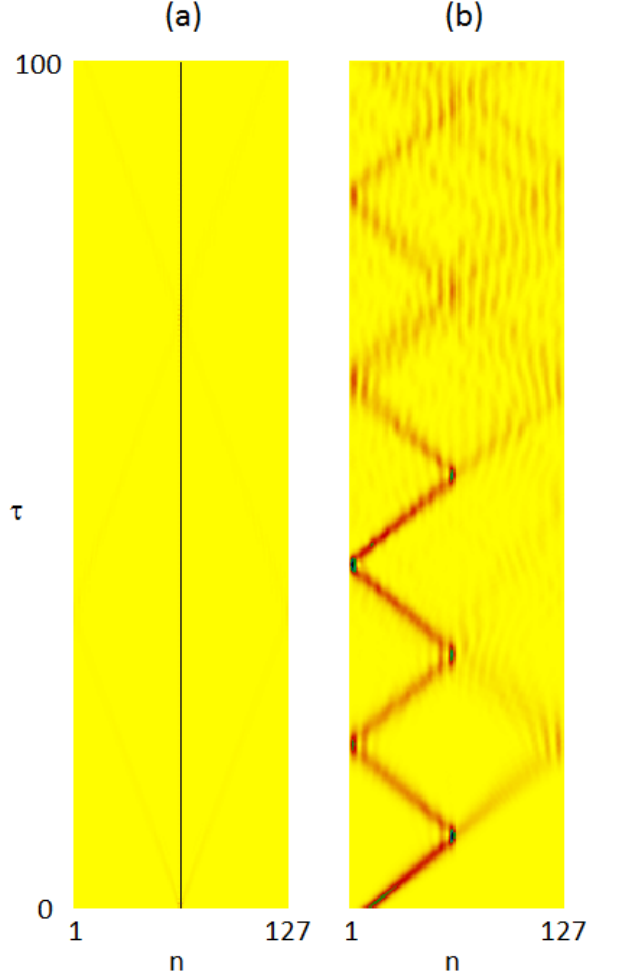


FIG. 9: (Color online) The same physical situation as in Fig. 8 but with  $\Lambda_{1,2} = -9$ . The traveling breather bounces elastically from the self-trapped state with only a minor proportion tunneling through.

trapped inside the other. Moreover, the breathers appear to accelerate or decelerate for a brief time during the strong interaction.

Quite different results are obtained for the  $^{41}\text{K} + ^{87}\text{Rb}$  mixture, characterized by a large tunneling rate ratio of  $\gamma_2/\gamma_1 \approx 6.97$ . This, together with the large self-interaction of Rb, changes the physics dramatically.

In Figs. 8 and 9 we show a collision of a traveling breather and a self-trapped state of rubidium atoms. Within the range of our simulation parameters that simulates possible experimental realizations, it has proved not possible to initiate a traveling breather state with the Rb condensate due to its large self-interaction. We set the interspecies interaction parameter  $\Lambda_{1,2} = 3$  for Fig. 8 and  $\Lambda_{1,2} = -9$  for Fig. 9. In both cases the rubidium breather acts only as a potential barrier, through which some of the incoming potassium soliton can either reflect or tunnel. This behavior, which contrasts with the phenomena seen in the simulation with ytterbium, can be attributed to the drastically different tunneling rates of potassium and rubidium.



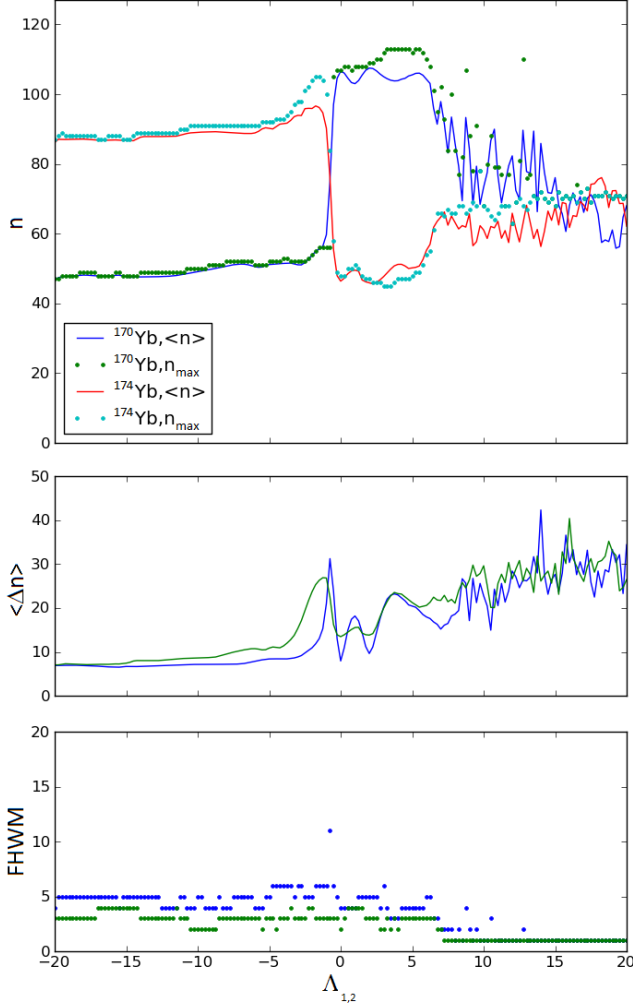


FIG. 10: (Color online) The collision outcome as a function of the interspecies interaction,  $\Delta_{1,2}$ . The top panel displays the mean and the peak site per species, the center panel the standard deviation per species, and the bottom panel the FWHM per species as defined in the text. Symplectic simulations corresponding to the  $^{170}\text{Yb}+^{174}\text{Yb}$  mixture.

## V. THE COLLISION MECHANISM

To understand the mechanisms at the base of the collision outcomes, we have investigated the dependence of the result of the collisional process with respect to the heteronuclear interaction. By treating the discrete condensate wavefunctions as distributions we define the mean lattice site

$$\langle n_i \rangle = \sum_n n |z_{i,n}|^2, \quad (16)$$

and its standard deviation,

$$\langle \Delta n_i \rangle = \left( \sum_n (n - \langle n_i \rangle)^2 |z_{i,n}|^2 \right)^{1/2}. \quad (17)$$

These two parameters describe the *global* behavior of the condensate. In fact, if a breather splits or is destroyed in a colli-

sion, the standard deviation increases dramatically. To assess the *local* behavior, i.e. looking for a new breather created in a collision, we also search for the site with the largest number of atoms,  $n_{\max,i}$  and attempt to estimate the new breather's width (Full Width Half Maximum, FWHM) by counting the adjacent sites which contain at least half the number of atoms of those in the site of the maximum.

Figure 10 shows the parameters  $\langle n_i \rangle$ ,  $n_{\max,i}$ ,  $\langle \Delta n_i \rangle$  and the FWHM as a function of the mutual interaction parameter  $\Delta_{1,2}$ . For each value of  $\Delta_{1,2}$  a simulation was performed up to  $\tau = 150$ , just past the collision. The initial conditions and interaction parameters are the same as in Fig. 4, except for the scanned  $\Delta_{1,2}$  and the tunneling ratio  $\gamma_2/\gamma_1$ , which is set to 1.

Four different regimes can be identified from Fig. 10. On the left, for  $\Delta_{1,2}$  lower than about  $-2.0$ , two traveling breathers collide elastically and remain basically unaffected by the collision. This is the situation shown in figure 4. Then, there is a transition point at  $\Delta_{1,2} \approx -1.5$  where the each breather splits into two as they collide. This results in a sudden increase of  $\langle \Delta n \rangle$  for each species. Note that this increase differs between the two species; for  $^{174}\text{Yb}$  it's maximum is located at  $\Delta_{1,2} \approx -2$  as opposed to  $\Delta_{1,2} \approx -1$  for  $^{170}\text{Yb}$ , quite probably as a result of the different self-interaction parameters.

For small, but positive values of  $\Delta_{1,2}$  (i.e. less than 6) the two breathers tunnel through each other. Note that  $\langle \Delta n \rangle$  remains low in this regime (about 15 sites, growing slowly to 20) which means that the breathers are not destroyed. This is shown in Fig. 7 for  $\Delta_{1,2} = 4$ . As the two breathers tunnel through each other, a part of their wavefunction is trapped inside the other soliton; this effect grows as the interspecies interaction increases leading to a slow increase in the standard deviation of the atomic density distributions.

A rather sudden change takes place at about  $\Delta_{1,2} = 6$ . The system becomes visibly sensitive to small changes in the mutual interaction. This is the regime where the collision results in the destruction of the two breathers. Fig. 6 is an example of such a case. The process is chaotic, yet in many cases leads to the creation of a double-species symbiotic breather manifested by its very low FWHM.

## A. Discussion

The presented results can be reasonably explained by using one of the key phenomena at the base of gap solitons: the *negative effective mass*. The dynamics of a gap soliton in an external potential are exactly opposite to what one would expect - a gap soliton attempts to climb potential hills and in itself is a balance between its negative effective mass that tries to make it collapse and its repulsive self-interaction that prevents it [11, 27]. In fact, the variational model of a wavepacket used in Trombettoni *et al.* [11] shows that the wavepacket center obeys a Newton-like dynamics when  $p \approx 0$  and exactly the contrary when  $p \approx \pi$ .

This 'contrary' behavior of the solitons seems to be the key to the explanation of our findings. The totally elastic collision encountered when the interspecies interaction is highly *attractive* would be caused by the fact that the solitons 'see'

each other as potential walls rather than wells.

The splitting behavior has been investigated in a slightly different context by Matuszewski *et al.* [27] where the dynamics of two already overlapped stationary solitons was analyzed. In our case splitting happens if the attractive interaction is small enough to let the two breathers overlap briefly. Then the system becomes unstable and each breather splits in two. It is also possible to look at this phenomenon from a different angle. Due to its negative effective mass, the split of the breather is quite similar to the case of a wavepacket encountering a potential barrier where, depending on the barrier height (or the interaction between the breathers) part of the wavepacket goes through while the rest is reflected.

In the repulsive interaction regime the breathers behave as if they saw each other as potential wells. This is again an effect of their negative effective mass and, consequently, reversed dynamics. Thus, for the collision's duration, their speed increases (at the cost of wavepacket spreading and of reducing their energy due to atomic self-interaction).

The chaotic behavior when the interspecies interaction is large and repulsive is probably caused by the system entering an unstable regime as predicted by Gubeskys *et al.* [24]. The chaotic dynamics would then cause the destruction of the original two breathers and possibly the creation of a stable *intragap* soliton. It is beyond the capabilities of our model to establish if it is possible for an *intergap* soliton to emerge during the collision since the tight-binding approximation is limited to the lowest band-gap by definition.

## VI. CONCLUSION

We have analyzed the behavior of interacting and colliding discrete breathers in BEC composed of different atomic species in optical lattices. We have found that the interaction depends on the initial distance of the two breathers and led either to the formation of a symbiotic solitons or to the setup in motion of one of the two breathers. The collision outcome depends both on the tunneling rate ratios of the two species, as well as the interspecies interactions. When the tunneling rates

differ greatly, as in the  $^{41}\text{K}+^{87}\text{Rb}$  mixture, one of the breathers acts as an effective potential wall to the other and the whole process can be viewed as a case of one-particle scattering on a potential wall.

In the case where the tunneling rates are comparable (like in the case of mixtures of Ytterbium isotopes) we have identified four collision regimes. For large negative scattering lengths the collision is elastic and the two traveling breathers remain intact, with considerable momentum transfer between the two. For small negative scattering rates, the breathers overlap briefly and split in two, as originally predicted in [27]. When the interspecies interaction is weakly repulsive, the two breathers tunnel through each other unharmed for a wide range of interspecies interactions. Finally, with the interspecies interaction sufficiently large, the dynamics becomes chaotic and the two breathers are destroyed with a possible creation a new two-component soliton similar to an *intragap* soliton as predicted in [24]. Feasible explanations to the above phenomena have been provided using the concept of negative effective mass and the resulting reversed dynamics.

Interaction and collision properties of localized excitations in BEC in optical lattices can have interesting applications in the realization of ultracold Bose-Fermi mixtures where gap solitons can be viewed as matter-wave counterparts of quantum dots and antidots [56]. Changing the species interaction allows one to tune the character of the collisions from fully elastic to fully inelastic and/or tunneling with clear advantages in the manipulation of information in matter-wave systems.

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